A Lattice Boltzmann Subgrid Model for High Reynolds Number Flows

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Abstract

A subgrid turbulence model for the lattice Boltzmann method is proposed for high Reynolds number fluid flow applications. The method, based on the standard Smagorinsky subgrid model and a single-time relaxation lattice Boltzmann method, incorporates the advantages of the lattice Boltzmann method for handling arbitrary boundaries and is easily implemented on parallel machines. The method is applied to a two-dimensional driven cavity flow for studying dynamics and the Reynolds number dependence of the flow structures. The substitution of other subgrid models, such as the dynamic subgrid model, in the framework of the LB method is discussed.

1 Introduction

The lattice Boltzmann (LB) method[1, 2, 3, 4, 5, 6, 7], a derivative of lattice gas automaton method[8, 9], has been successfully demonstrated to be an alternative numerical scheme to traditional numerical methods for solving partial differential equations and modeling physical systems, particularly for simulating fluid flows with the Navier-Stokes equations. In traditional numerical methods, a given set of macroscopic equations are solved by some specific numerical discretization. In contrast, the fundamental principle of LB method is to construct a simplified molecular dynamics that incorporates the essential characteristics of the physical microscopic processes so that the macroscopic averaged properties obey the desired macroscopic equations. This microscopic approach in the LB method incorporates several advantages of kinetic theory. It includes clear physical pictures, easy implementation of boundaries and fully parallel algorithms. In particular, the LB method has been successfully applied to problems which are usually difficult for traditional numerical schemes, such as fluid flows through porous media[10, 11], multiphase fluid flows[12, 13, 14, 15, 16, 17] and suspension motions in fluids[18, 7].

The LB method so far has been used only as a direct numerical simulation method, *i.e.*, the full Navier-Stokes equations are directly solved without any *ad hoc* assumptions for constitutive relation between turbulence stress tensor and the mean strain tensor. Therefore, the smallest captured scale in the LB method is the lattice unit and the largest scale depends on the characteristic length scale in simulation. These scales are often determined by the available computer memory. The LB method is consequently able to resolve relatively low Reynolds number flows. It should be noted that although the LB method greatly reduces noise of a system compared with lattice gas schemes, the lattice Boltzmann method can become numerically unstable in contrast with lattice gas methods, where the scheme is unconditionally stable. Numerical studies have shown that the using of the LB method for high Reynolds number flows, without modeling unresolved small scale effects on large scale dynamics, results in numerical instability. This result is consistent with the recent argument made by Sterling and Chen[19] that the LB method can be viewed as an explicit second-order finite-difference discretization scheme. The objective of this paper is to provide a numerical method based on the LB method which can simulate fluid flows at high Reynolds numbers with large eddy dynamics.

There are two ways to extend the LB method to include small scale dynamics for high Reynolds number flows. First, since the LB method was originated from lattice gas automaton method and the lattice gas dynamics contains small scale fluctuations intrinsically, it is natural to consider a hybrid method, in which the LB method is used for large scale motions and the lattice gas method is used to simulate small scale dynamics, *i.e.*, at each point in lattice Boltzmann space, one allows a sublattice to evolve according to lattice gas rules[21]. Unfortunately, no progress has been made

using this approach so far. The fundamental difficulty there is to incorporate the interaction between small scale dynamics and large scale dynamics using a microscopic particle picture. A simpler approach is to combine the traditional subgrid model with a LB method. Some early work by Benzi *et al.*[6] and recent work at Los Alamos National Laboratory[20] and by Qian *et al.*[22] follow this approach. This research has helped to motivate our current studies.

Numerical simulation using a subgrid model for the Navier-Stokes equations by traditional numerical methods is still an open and difficult problem. The basic idea of all subgrid models is to make use of an assumption to include the physical effects that the unresolved motion has on the resolved fluid motion. These models often take a simple form of eddy-viscosity models for the Reynolds stress that serve to damp short-wavelength oscillations. Among the simplest subgrid models is the standard Smagorinsky model[23], which uses a positive eddy viscosity to represent small scale energy damping. However, recent research by several groups[24] has demonstrated that the eddy-viscosity acting on scales smaller than some applied test grid could be large and positive at some locations and large and negative at others. The standard subgrid model cannot represent these "backscatter" phenomena. Recent development of dynamic subgrid models[24] represent the current trend to include dependence of the subgrid model coefficients on local quantities to account for these effects.

From the numerical analysis point of view, the subgrid model must provide a stable numerical scheme. On the other hand, stable numerical schemes contain some artificial dissipation and/or dispersion. One basic question to be answered is whether a solution using a stable numerical scheme can represent the energy transfer between large and small scales effcetly as a subgrid model.

The present paper neither aims to develop a new subgrid model nor discusses the relation between the subgrid model and numerical stability. We will simply demonstrate that the traditional subgrid model can be easily incorporated into the framework of the LB method. The scheme developed here can be easily extended to include the dynamic subgrid model and others[24]. To illustrate how to use the lattice Boltzmann subgrid model, we will present simulation results for a driven cavity flow at Reynolds numbers varying from 100 to 1 million based on the physical viscosity.

2 Lattice Boltzmann Method and Single-Time-Relaxation-Approximation

In the LB method, the evolution equation for the particle distribution function, $f_i(\mathbf{x}, t)$, can be written as follows,

$$f_i(\mathbf{x} + \mathbf{e}_i, t + 1) = f_i(\mathbf{x}, t) + \Omega_i(f(\mathbf{x}, t)), \tag{1}$$

where $\Omega_i = \Omega_i(f(\mathbf{x}, t))$ is a local collision operator depending on local particle distribution f_i only. The velocity vectors are $\mathbf{e}_i$, where $i = (0, 1, \cdots, b)$ and b is the number

of the nearest neighbors. b equals to 6 for a hexagonal lattice and 8 for a square lattice. The above lattice Boltzmann equation can be obtained from two different ways: First, the lattice Boltzmann equation can be naturally derived from the lattice gas equation for particle occupation, N_i, by assuming no particle-particle correlations, where N_i is a Boolean variable. Although equation (1) has been written down earlier by several people[8, 9] to derive the asymptotic behavior of the lattice gas, it was first proposed by McNamara and Zanetti[1] to use (1) as a direct numerical method, where they simply replace N_i by f_i in the lattice gas automaton equation[8] without changing the collision operator and streaming steps. This produces: $\langle N_i \rangle = f_i$ and $\langle \Omega_i(N(\mathbf{x}, t)) \rangle = \Omega_i(f(\mathbf{x}, t))$, where $\langle\rangle$ denotes an ensemble average. Second, if one starts from a continuum kinetic equation for particle distribution function, f_i,

$$\frac{\partial f_i}{\partial t} + \mathbf{e}_i \cdot \nabla f_i = \Omega_i, \tag{2}$$

then the lattice Boltzmann equation in (1) can be regarded as a Lagrangian solution using an Euler time step in conjunction with an upwind spatial discretization[19]:

$$\frac{f_i(\mathbf{x}, t + \Delta t) - f_i(\mathbf{x}, t)}{\Delta t} + \frac{f_i(\mathbf{x} + \mathbf{e}_i \Delta x, t + \Delta t) - f_i(\mathbf{x}, t + \Delta t)}{\Delta x} = \Omega_i. \tag{3}$$

Upon setting the time spacing equal to grid spacing (particle with lattice speed), equation (3) becomes the same as (1).

An important refinement of the LB method proposed by Higuera and Jimenez [2] was to replace the "exact" collision operator by a linearized collision operator. A further simplification for the collision operator was offered nearly simultaneously by two groups[3, 4, 25]. They assumed that the exact collision operator can be discarded, provided one adopts a collision operator that leads, in a controllable fashion, to a desired local equilibrium state. They chose an equilibrium distribution function that depends only upon the local fluid variables, which can be computed from the actual values of the local distribution at a point and which leads to the desired macroscopic equations.

For developing a magnetohydrodynamic (MHD) lattice Boltzmann method, Chen *et al.*[3] offered the first suggestion that one could further simplify the collision operator by using a single-time-relaxation approximation, or STRA. Subsequently, a similar method[4] was described, and referred to as a "BGK" collision integral, in reference to the more elaborate collision treatment of Bhatnagar, Gross and Krook[26]. The essence of the suggestion for the LB method is that the collision term, $\Omega(f)$, be replaced by the well-known single-time-relaxation approximation, $\Omega(f) = -\frac{f - f^{eq}}{\tau}$. The appropriately chosen equilibrium distribution is denoted by f^{eq} and depends upon the local fluid variables. A lattice relaxation time, τ, controls the rate of approach to equilibrium. Later, Qian *et al.*[4] and Chen *et al.* [25] described an STRA method for hydrodynamics that incorporates a rest particle state in order to be consistent with the exact Navier-Stokes equations.

To derive the Navier-Stokes equations, the Chapman-Enskog procedure is utilized, assuming the following multi-scale expansion of the time and space derivatives in the small parameter, ϵ:

$$\frac{\partial}{\partial t} = \epsilon \frac{\partial}{\partial t_1} + \epsilon^2 \frac{\partial}{\partial t_2} + ...,$$
$$\nabla = \epsilon \nabla_1 + \epsilon^2 \nabla_2 + \cdots. \tag{4}$$

We also expand the distribution function as

$$f_i = f_i^{(0)} + \epsilon f_i^{(1)} + \epsilon^2 f_i^{(2)} + \cdots, \tag{5}$$

where the zeroth-order term is the equilibrium distribution function, so that the collision operator becomes

$$-\frac{(f_i - f_i^{eq})}{\tau} = -\frac{1}{\tau}(f_i^{(1)} + \epsilon f_i^{(2)} + ...). \tag{6}$$

Note that the parameter ϵ can be regarded as a Knudsen number similar to kinetic theory in classical statistical mechanics. Since the mass, n, and the momentum, $n\mathbf{u}$, are conserved in collisions:

$$n = \sum_i f_i = \sum_i f_i^{(0)}, n\mathbf{u} = \sum_i f_i \mathbf{e}_i = \sum_i f_i^{(0)} \mathbf{e}_i,$$

the summations over nonequilibrium populations are zero: $\sum_i f_i^{(l)} = 0$ and $\sum_i \mathbf{e}_i f_i^{(l)} = 0$ for $l > 0$.

Substituting the above expansions into (1), we obtain equations of first and second order in ϵ which are written as

$$\frac{\partial}{\partial t_1} f_i^{(0)} + \mathbf{e}_i \cdot \nabla_1 f_i^{(0)} = -\frac{1}{\tau} f_i^{(1)}, \tag{7}$$

and

$$\frac{\partial f_i^{(0)}}{\partial t_2} + (\frac{\partial}{\partial t_1} + \mathbf{e}_i \cdot \nabla_1)(1 - \frac{1}{2\tau}) f_i^{(1)} = -\frac{f_i^{(2)}}{\tau}. \tag{8}$$

where τ is assumed to be $O(1)$.

When equations (7) and (8) are summed over the i velocities, the continuity or mass conservation equation to second order in ϵ is

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{u}) = 0. \tag{9}$$

The momentum equation to second order in ϵ is obtained by multiplying the above equations by $\mathbf{e}_i$ and then summing over velocities,

$$\frac{\partial}{\partial t}(n\mathbf{u}) + \nabla \cdot (\mathbf{\Pi}^{(0)} + (1 - \frac{1}{2\tau})\mathbf{\Pi}^{(1)}) = 0, \tag{10}$$

where $\mathbf{\Pi}^{(0)}$ and $\mathbf{\Pi}^{(1)}$ are the momentum flux tensors, defined as

$$\mathbf{\Pi}^{(0)}_{\alpha\beta} = \sum_i e_{i\alpha} e_{i\beta} f_i^{(0)}, \tag{11}$$

and

$$\mathbf{\Pi}^{(1)}_{\alpha\beta} = \sum_i e_{i\alpha} e_{i\beta} f_i^{(1)}. \tag{12}$$

Note that the factor $\frac{1}{2\tau}$ comes from the second time and space derivatives[7].

The constitutive relations for this tensor are obtained by selecting a particular lattice geometry and equilibrium distribution functional form and then proceeding to match moments of the distribution function with terms in the Navier-Stokes equations.

As an example, we use in this paper a 9-velocity square lattice with velocity vectors, $\mathbf{e}_i^I = \{cos(\pi(i-1)/2), sin(\pi(i-1)/2)\}$ and $\mathbf{e}_i^{II} = \sqrt{2}\{cos(\pi(i-\frac{1}{2})/2), sin(\pi(i-\frac{1}{2})/2)\}$ for $i = 1, \cdots, 4$. A suitable equilibrium distribution function is found to be

$$\begin{aligned} f_0^{\mathrm{eq}} &= \frac{4}{9} n[1 - \frac{3}{2}u^2], \\ f_i^{I,\mathrm{eq}} &= \frac{n}{9}[1 + 3\mathbf{e}_i^I \cdot \mathbf{u} + \frac{9}{2}(\mathbf{e}_i^I \cdot \mathbf{u})^2 - \frac{3}{2}u^2], \\ f_i^{II,\mathrm{eq}} &= \frac{n}{36}[1 + 3\mathbf{e}_i^{II} \cdot \mathbf{u} + \frac{9}{2}(\mathbf{e}_i^{II} \cdot \mathbf{u})^2]. - \frac{3}{2}u^2. \end{aligned} \tag{13}$$

Substituting equation (13) into equation (10) for $\mathbf{\Pi}$ above and noting the velocity moment relations on the square lattice[7], we find that

$$\mathbf{\Pi}^{(0)}_{\alpha\beta} = \frac{n}{3}\delta_{\alpha\beta} + n u_\alpha u_\beta.$$

This provides a Galilean invariant convective term in the momentum equation. By identifying the isotropic part of this tensor with the pressure, we obtain an ideal gas equation of state (*i.e.* $p = \frac{n}{3}$).

Neglecting terms of order u^3 and higher, we have:

$$\mathbf{\Pi}^{(1)}_{\alpha\beta} = -(\tau - \frac{1}{2})\{\frac{\partial}{\partial t}\mathbf{\Pi}^{(0)}_{\alpha\beta} + \frac{\partial}{\partial x_\gamma}\sum_i e_{i\alpha} e_{i\beta} e_{i\gamma} f_i^{(0)}\}.$$

From the distribution function in (13)[28], we have:

$$\mathbf{\Pi}^{(1)}_{\alpha\beta} = -\frac{2n\tau}{3} S_{\alpha\beta}, \tag{14}$$

with $S_{\alpha\beta} = \frac{1}{2}(\frac{\partial u_\beta}{\partial x_\alpha} + \frac{\partial u_\alpha}{\partial x_\beta})$.

Upon substitution into equation (10), the final form of the momentum equation is

$$n\frac{\partial u_\alpha}{\partial t} + nu_\beta\frac{\partial u_\alpha}{\partial x_\beta} = -\frac{\partial p}{\partial x_\alpha} + \frac{\partial}{\partial x_\beta}(\mu(\frac{\partial u_\beta}{\partial x_\alpha} + \frac{\partial u_\alpha}{\partial x_\beta})), \tag{15}$$

where μ is the shear viscosity,

$$\mu = \frac{(2\tau - 1)n}{6}, \tag{16}$$

and this gives a kinematic viscosity of $\nu = \frac{(2\tau-1)}{6}$.

There are differences between the incompressible Navier-Stokes equations and the macroscopic behavior of the discrete-velocity Boltzmann equations derived above because of the asymptotic nature of the Chapman-Enskog method. The differences may be attributed to two causes: 1) Burnett level and higher level terms or as small deviations from the above relation for the kinematic viscosity; 2) high order velocity terms[27] and compressibility effects. Since the Knudsen number is proportional to the Mach number divided by the Reynolds number, the Burnett terms may be classified with other "compressibility" effects and should become small as the Mach number approaches zero for a fixed Reynolds number.

The particle interpretation of the LB method allows boundary conditions to be implemented as particular types of collisions. If populations are reflected directly back along the lattice vector from which they came, the result is a "no-slip" velocity boundary condition. One may also define specular reflection conditions that yield a slip condition. These simple boundary conditions make the LB method particularly suited to parallel computing environments and the simulation of flows in complex geometries. It should be mentioned, however, that the recent work by Hou *et al.*[28]has demonstrated that even though the LB method discussed above is of second order accuracy for both space and time discretization, the simple particle bounce back leads to a first order accuracy in spatial discretization at the boundary. Nevertheless, second order schemes similar to bounce back have been proposed recently by Skordos[29] and Noble *et al.*[30].

Since the LB method under consideration is valid only in the incompressible limit, the main dimensionless parameter of interest is the Reynolds number. Here the Reynolds number is defined as,

$$Re = \frac{LU}{\nu} = \frac{6NU}{\tau - \frac{1}{2}},$$

where $N = \frac{L}{\Delta x}$ is the number of lattice spaces and U is a characteristic velocity. Convergence of the solution to the incompressible Navier-Stokes equations for a fixed Reynolds number is then obtained by letting the Mach number become small enough to remove compressibility effects, and letting the lattice spacing $\mathbf{e}_i\Delta t$ become small enough to resolve the flow. Several recent studies have shown[28, 31, 32] that the

lattice Boltzmann methods accurately predict incompressible fluid flows in this limit. Moreover, the convergence at a fixed Reynolds number is performed by increasing N while either increasing τ and/or decreasing U appropriately. For a decrease in the value of U, a proportionate increase in the number of time steps is needed to reach the same flow evolution time.

3 The Lattice Boltzmann Subgrid Model

To simulate large scale resolved fluid problems at high Reynolds numbers, a space filtering operation is often introduced,

$$\overline{w}(x) = \int w(x) G(x, x') dx', \tag{17}$$

where w can be density, velocity or any other physical quantity; G is a given spatial filter function and the integral is extended over the entire domain. Several different filters[33] can be used, depending on the numerical method in use. For most finite difference methods, the box filter is assumed and is defined as follows:

$$G_i(x_i, x_i') = \begin{array}{c} \frac{1}{\Delta_i} for\, |x_i - x_i'| < \frac{\Delta_i}{2}, \\ 0 otherwise, \end{array} \tag{18}$$

while for spectral methods, a cutoff filter defined in Fourier space is used,

$$\widehat{G}_i(k_i) = \begin{array}{c} 1 for k_i < K_i \\ 0 otherwise, \end{array} \tag{19}$$

where $\widehat{G}_i$ is the Fourier coefficient of the filter function in the ith direction, G_i, $K_i = \pi/\Delta_i$ is the cutoff wavenumber, and Δ_i is the filter width in the ith direction. Applying the same filtered operation to density, pressure and velocity in equation (9) and (15) in the incompressible limit, it can be easily shown that the filtered continuity and momentum equations are

$$\begin{array}{c} \frac{\partial \overline{u}_i}{\partial x_i} = 0 \\ \frac{\partial \overline{u}_i}{\partial t} + \overline{u}_j \frac{\partial \overline{u}_i}{\partial x_j} = -\frac{1}{n}\frac{\partial \overline{p}}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} + \frac{\partial}{\partial x_j}\left(\nu\left[\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}\right]\right), \end{array} \tag{20}$$

where τ_{ij} is the Reynolds stress, representing the effects of the unresolved scales on the resolved scales:

$$\tau_{ij} = \overline{u_i u_j} - \overline{u}_i \overline{u}_j \tag{21}$$

These equations govern the evolution of the resolved fluid motions. For laminar flows, today's computational power is often adequate to resolve all scales, which in the context of filtering simply means that τ_{ij} is negligible. For turbulent flows, however, the Reynolds stress is significant and must be modeled in some way. The use of

artificial dissipation or dispersion in any numerical schemes to stablize the solution is equivalent to setting discretization error equal to this Reynolds stress term. Thus, any numerical viscosity will effectively serve as a subgrid turbulence model. The main criterion for stability of numerical methods is that this term effectively damps short-wavelength oscillations in the flow.

The most common approach to subgrid modeling is due to Smagorinsky [23] in which the anisotropic part of the Reynolds stress term is modeled as

$$\tau_{ij} - \frac{\delta_{ij}}{3}\tau_{kk} = -2\nu_t \overline{S}_{ij} = -2C\Delta^2 \left|\overline{S}\right| \overline{S}_{ij}, \tag{22}$$

in which δ_{ij} is the Kronecker delta function and $\left|\overline{S}\right| = \sqrt{2\overline{S}_{ij}\overline{S}_{ij}}$ is the magnitude of the large scale strain rate tensor

$$\overline{S}_{ij} = \frac{1}{2}\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}\right). \tag{23}$$

and $C > 0$ is the Smagorinsky constant. The isotropic part of the Reynolds stress term can be included in the pressure term.

A recent modification to this model by Germano *et al.* [24] is called the dynamic subgrid eddy viscosity model and applies a test filter in addition to the grid filter. The so-called "resolved Reynolds stress" terms that are computed for scales between the coarse test filter and the grid filter can then be used to locally compute the Smagorinsky constant, C. A problem with this model, however, is that the Smagorinsky constant may become locally negative and numerical instability ensues. This is avoided in practice by averaging over homogeneous flow planes to keep positive eddy viscosities or by developing even more sophisticated and more complicated models.

The fundamental question we are facing is how to modify the lattice Boltzmann method discussed in the previous section to simulate the filtered density and velocity in equation (15). In order to apply the subgrid idea in the framework of LB method, let us introduce the filtered particle distribution, $\overline{f}_i$, defined as follows:

$$\overline{f_i}\,(x) = \int f_i\,(x)\, G\,(x, x')\, dx',$$

and modify the microscopic equation (2) to be a kinetic equation for the filtered particle distribution function:

$$\frac{\partial \overline{f}_i}{\partial t} + \mathbf{e}_i \cdot \nabla \overline{f}_i = \overline{\Omega}_i. \tag{24}$$

Using the finite-difference scheme in (3) for (24), we will obtain similar equation in (1) for $\overline{f}_i$.

There are two possible approaches. First, one can use the unfiltered equilibrium distribution (1) as the fundamental equation. When we apply the G-filter on the collision term, or the equilibrium distribution function, we obtain several correlation terms due to the nonlinearity of velocity in the equilibrium distribution function: $\overline{nu_\alpha}$ and $\overline{nu_\alpha u_\beta}$, which need to be closed. Therefore, the closure problem is again encountered. It can be argued that these particle-particle space correlations may be easier to model using physical arguments based on microscopic simplicity. The final results of modeling these terms should be equivalent to modeling the Reynolds stress at the macroscopic level.

A second and more direct approach is to link the collision steps with some local information and abandon the single-time-relaxation approximation. To do this, we assume that the filtered particle distribution will approach a local filtered equilibrium distribution, which can be chosen to depend only on local filtered mean quantities, $\overline{n}$ and $\overline{\mathbf{u}}$, *i.e.*, $\overline{\Omega_i(f(\mathbf{x},t))} = \Omega_i(\overline{f(\mathbf{x},t)})$ and the form of the equilibrium distribution function are all the same as in (13), except now we will use the filtered quantities to replace the unfiltered quantities. In addition, we further assume that the effect of the correlation will only locally introduce an eddy viscosity and we allow the relaxation time to depend on space. Explicitly, we will incorporate the Smagorinsky formula for eddy viscosity into the relaxation time, τ. Since in the LB method, the lattice spacing is set to 1, the relaxation time is equivalent to the mean free path of a particle. The above arguments can be directly linked to the early idea in Prandtl's mixing length theory[34], *i.e.* the change of relaxation time can be equivalently interpreted as a change in the local mean free path and therefore the local viscosity.

It can be easily proved that the spatial dependence of the relaxation time, τ, will not change the Chapman-Enskog expansion procedure and does not affect the derivation of the Navier-Stokes equations in the last section. That means equations (9) and (15) can also be derived using equation (24), assuming: $\overline{n} = \sum_i \overline{f}_i$ and $\overline{n}\overline{\mathbf{u}} = \sum_i \overline{f}_i \mathbf{e}_i$. We also find that if the total viscosity equals the sum of the physical and the eddy viscosities (the Smagorinsky model),

$$\nu_{total} = \nu_0 + C\Delta^2 \left|\overline{S}\right|, \tag{25}$$

where ν_{total} is the total viscosity; ν_0 is the physical kinematic viscosity and $C\Delta^2 \left|\overline{S}\right|$ is the eddy-viscosity term, we should let the relaxation time, τ, be a function of total viscosity. Using (16), we have,

$$\frac{2\tau_{total} - 1}{6} = \nu_{total},$$

and we obtain a simple relation:

$$\tau_{total} = 3\nu_{total} + \frac{1}{2},$$

or

$$\tau_{total} = 3(\nu_0 + C\Delta^2 \left|\overline{S}\right|) + \frac{1}{2}.$$

Thus, the value of τ should be locally adjusted, depending on the local magnitude of the large scale strain rate tensor. The dynamic eddy viscosity model may also be implemented by using the local value of C that is computed from the resolved Reynolds stress term using the test filter[24].

It should be mentioned that the calculation of local intensity of the strain tensor can be easily carried out using the nonequilibrium properties of the filtered particle distribution. The procedure is:
(a) calculate locally the nonequilibrium stress tensor:

$$\overline{\Pi}_{i,j} = \sum_{\alpha} \mathbf{e}_{\alpha i}\mathbf{e}_{\alpha j}(\overline{f}_i - \overline{f}_i^{eq});$$

(b) calculate the second variance of the tensor $\Pi_{i,j}$, $\mathrm{Q} = \overline{\Pi}_{i,j}\overline{\Pi}_{i,j}$;
(c) neglecting high order velocity effects and using equation (14), we prove that the following relation is valid:

$$Q^{1/2} = (\tau_0 + 3C\Delta^2|\overline{S}|)\frac{2n}{3}|\overline{S}|, \tag{26}$$

where $|\overline{S}|$ is the intensity of the local filtered strain tensor and $\tau_0 = 3\nu_0 + \frac{1}{2}$. Solving the above equation for $|\overline{S}|$, we have:

$$|\overline{S}| = \frac{\sqrt{\nu_0^2 + 18C\Delta^2 Q^{1/2}} - \nu_0}{6C\Delta^2}.$$

The solution through the above equation guarantees the required positivity of $|\overline{S}|$.

In a traditional scheme, a finite difference must be used for calculating the local strain tensor. In the present model, the strain tensor can be calculated locally using the nonequilibrium distribution. This simple procedure should save considerable computational time.

4 Turbulence Structures in a Driven Cavity Using a Lattice Boltzmann Simulation

The two-dimensional driven cavity flow considered here is used as a testbed for the subgrid model described above. The incompressible fluid is bounded in a square enclosure. The flow is driven by the uniform translation of the top boundary. The flow configurations generated in this cavity show rich vortex phenomena at many scales depending on the Reynolds number, Re. Cavity flow has been used extensively

in various numerical schemes as an ideal problem for studying complex flow physics in a simple geometry.

Most numerical solutions of two-dimensional cavity flow use a vorticity-stream function formulation and discretize the incompressible, steady linear or nonlinear Navier-Stokes equations by finite difference, finite element methods or their combinations with multigrid and other methods. Among the previous research, Ghia *et al.* [35] obtained numerical solutions up to Re=10,000 with a 257×257 grid. Their work represents the most comprehensive study of 2-D cavity flow to date.

The cavity flow using the lattice Boltzmann method without subgrid model are studied carefully by Hou *et al.*[28]. Detailed quantitative comparisons between the LB and traditional methods for laminar flow (Re $\leq$ 7500) were carried out. The compressibility error and the convergence rate of the method, as well as parameter ranges for stable simulations are also explored in that paper. The results obtained by LB method compared well with Ghia *et al.* [35]. The maximum and minimum values of stream function for primary and secondary vortices agree with each other within 0.2 % for all values of Re tested. The locations of the vortex centers predicted by the lattice Boltzmann method also agree well with those given by Ghia *et al.* [35].

Most previous finite-difference or finite-element methods are only concentrated in steady-state behavior and therefore only the steady-state, partial differential equations are used. In contrast, the LB method is a direct numerical scheme based on the unsteady microscopic kinetic equation. The time dependent behavior will be calculated in spite of the time-dependent properties of the flow. In some sense, the LB method is close to a time-dependent method in traditional finite schemes. It is quite encouraging that even though the LB method is very different from other traditional methods from lots of aspects, including microscopic vs. macorscopic and time-dependent vs. time-independent, the dynamic properties of the flow agree each other surprisingly well. Nevertheless, it should be realized that the highest Re number for a cavity flow is limited about 10,000 using a LB method without subgrid model on a 256×256 lattice. If viscosity is decreased further to increase Re, the computational instability will cause the simulation to blow up. At such a high Re, flows are turbulent. The value of Re can also be increased by increasing the number of lattice sites and increasing the maximum velocity. The former is limited by computer memory and the latter increases the compressibility error. It appears that the original lattice Boltzmann model is more adequate to laminar flow with low Reynolds numebr than to turbulent flow with high Reynolds number. The combination of the LB method with the subgrid model described in this paper allows simulations of cavity flow to reach up to a Reynolds number of 10^6.

The present simulation uses Cartesian coordinates with the origin located at lower left corner. The top wall moves from left to right with a uniform velocity, U. The cavity has 256 lattice units on each side. Initially, the velocities at all nodes, except the top, are set to zero. The x-velocity of the top is U and the y-velocity is zero. A uniform

initial particle density is imposed such that the moving particle along the $\mathbf{e}_i^I$ direction has a density fraction of $d = \frac{\overline{n}}{9} = 0.3$ per direction. The moving particle along the $\mathbf{e}_i^{II}$ direction has a density fraction of $\frac{d}{4}$, and the rest particle has a density of $4d$. Hence, the total density per node is $\overline{n} = 2.7$. Using the uniform density distribution and velocities given above, the equilibrium particle distribution function, $\overline{f}_i$, is calculated according to (13). The evolution of $\overline{f}_i$ can then be found by a succession of streaming and collision-like processes. After streaming, the velocity of the top lid is reset to the uniform initial velocity. After the streaming and collision process cycles, the particle distribution function, $\overline{f}_i$, at the top is set to the equilibrium state and bounce-back boundary conditions are used at the three stationary walls. The two upper corners are singular points which are considered as part of the moving lid in the simulations, but tests shown there is little difference if these two points are treated as fixed wall points. The uniform velocity of the top wall used in the simulations was U=0.1. The Reynolds number used in the cavity simulation is defined as Re =UL/ν, where U is the uniform velocity of the top plate, L is the edge length of the cavity and ν is the kinematic viscosity related to the single relaxation time as given in (16). All results are normalized to allow comparisons between the present work and other results based on a unit square cavity with unit velocity of the top boundary[35].

Steady-state solutions for cavity flow are obtained using the lattice Boltzmann method with subgrid model for Re=100, 2,000, and 7,500. The Re=10,000 case is also run on a 256×256 lattice, but steady state cannot be reached because bifurcation takes place somewhere between Re=7,500 and 10,000. The results for Re=10,000 oscillate between a series of different configurations. All of the results obtained by the present model for laminar flow ($Re < 7500$) agree well with that obtained by LB method without using subgrid model. Three Smagorinsky constants, *i.e.*, $C = 0.0025, C = 0.01$, and $C = 0.04$ are tested for these simulations. The two former cases give relatively smaller error for the velocity field. For $Re = 10^5$ and $Re = 10^6$, the Smagorinsky constant we are using is higher than the value quoted from other traditional schemes[24] and it cannot be lower than 0.073 and 0.084, respectively, otherwise the particle distribution function becomes negative, which means the eddy viscosity is not sufficient to damp the high-frequency fluctuations at small scales. It appears that the value of the Smagorinsky constant stongly depends on the geometry.

Figure 1 shows plots of the stream function for the Reynolds numbers considered. It is apparent that the flow structure is in good agreement with Ghia *et al.* for laminar flow. These plots give a clear picture of the overall flow pattern and the effect of Reynolds number on the structure of the recirculating eddies in the cavity. In addition to the central vortex, a pair of counterrotating eddies of much smaller strength develop in the lower corners of the cavity at Re=100. At Re=2000, a third secondary vortex is observed in the upper left corner. For Re ≥5,000, a tertiary vortex in the lower right hand corner appears. For $Re = 10^5$ and 10^6, a series of vortices are formed at the lower boundary. For low Re (*e.g.* Re=10, not shown here), the

center of the primary vortex is located at the midwidth and at about one third of the cavity depth from the top. As Re increases ($Re = 100$), the primary vortex center moves towards the right and becomes increasing circular. This center moves down towards the geometric center of the cavity as the Re increases and becomes fixed in its x location for Re $\geq$ 5,000. For turbulent flow the primary vortex is no longer round. In the case of $Re = 10^5$, the core of the primary vortex changes its shape and rotates with time. When the value of Re as high as 10^6, the vortex street is formed inside the primary vortex.

The plots of vorticity in Figure 2 show that the laminar cavity flow within closed streamlines at relative high Re consists of a central, inviscid core of nearly constant vorticity with viscous effects confined to thin shear layers near the walls. As Re increases, several regions of high vorticity gradients (indicated by concentration and wiggle of the vorticity contours) appear within the cavity. However, for turbulent flow there is no such inviscid core and a full developed turbulence is seen at $Re = 10^6$. Quantitative study of turbulence by present model is undertaken. Improvement of the subgrid model used in the lattice Boltzmann method is also needed.

5 Concluding Remarks

In this paper, we have presented a lattice Boltzmann subgrid model for simulating fluid flows at high Reynolds numbers. The essential idea is to define a space-filtered particle distribution and to allow the dynamics of the filtered particle distribution to have a space-dependent relaxation. This is equivalent to Prandtl's mixing length theory for which the mean free path of particle will be affected by the local strain intensity. The current model is able to incorporate the standard Smagorinsky subgrid model to include the energy dissipation induced by the interaction between resolved and unresolved scales. The lattice Boltzmann method proposed in this paper does not require calculation of the local strain intensity (nor the Reynolds stress tensor) using a finite difference scheme. Instead, the Reynolds stress is calculated locally at each time step using the nonequilibrium particle distribution functions. This additional advantage may allow the computational program to be more efficient than traditional finite different schemes.

The application of the current lattice Boltzmann model to a driven cavity fluid flows over a large range of Reynolds numbers has been carried out. The simulation results agree well with other methods for low Reynolds number fluid flows and qualitatively agree with previous simulations for high Reynolds numbers.

There are several issues to be addressed. First, to stablize numerical simulations, the current lattice Boltzmann subgrid model requires the Smagorinsky constant slightly bigger than the value commonly used in other geometries. This could be an indication of the geometry-dependence of the constant as observed in other finite difference simulations. It could also be attributed to the fact that the current

lattice Boltzmann method is only accurate to first order at the boundaries[28].

Second, it should kept in mind that the development of the lattice Boltzmann subgrid model is necessitated by a numerical instability encountered in lattice Boltzmann simulations at high Reynolds numbers. As mentioned in Section 1, the lattice gas automaton is unconditionally stable. Using real number manipulation in the LB method does reduce the noise and possibly utilizes memory more efficiently[7]. The real number operations introduce the same numerical round-off error and, therefore, instability problem encountered in other explicit finite different schemes. Moreover, the introduction of *ad hoc* assumptions in subgrid models can not be theoretically justified at the present time. The current subgrid models must be considered to be phenomenological. It is desirable that lattice gas models could simulate fluid flows with high Reynolds number. Unfortunately all known lattice gas models can only simulate relatively large viscosities, *i.e.* low Reynolds number. At the moment, it is not clear if the lattice Boltzmann subgrid model is better or worse than lattice gas model or other traditional finite difference schemes for simulating high Reynolds number flows.

Third, it appears that more careful quantitative comparisons between the lattice Boltzmann subgrid method and other numerical schemes are needed. These comparisons should include studies of numerical accuracy and computational speed. In addition, the current simulation only involves a simple geometry. It would be interesting to apply the current scheme to complicated geometries and to complicated physical phenomena, such as the multiphase fluid flows, for which the traditional schemes may have difficulties.

As a final remark, we emphasize that the current scheme can be extended easily to other dynamic subgrid models. Both the standard Smagorinsky model and the dynamic model of Germano *et al.* [24] have been implemented on the CM-5 computer at the Los Alamos Advanced Computing Laboratory to understand fluid instabilities and high Reynolds number flows[20]. It also should be pointed out that other possible subgrid models at the particle level, such as the model based on the first approach in the discussion of Section 3 may lead to more physically based turbulent models and could link the microscopic world with the macroscopic effective subgrid viscosity.

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7 Figure Captions

Fig. 1 Contour plots of the stream function at Re = 100, 2000, 7500, 10^4, 10^5 and 10^6.

Fig. 2 Contour plots of the vorticity distribution function at Re = 100, 2000, 7500, 10^4, 10^5 and 10^6.